Optimal control of the silicon-based donor electron spin quantum computing

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We demonstrate how gradient ascent pulse engineering optimal control methods can be implemented on donor electron spin qubits in Si semiconductors with an architecture complementary to the original Kane's proposal. We focus on the high-fidelity controlled-NOT (CNOT) gate and explicitly find its digitized control sequences by optimizing its fidelity over the external controls of the hyperfine A and exchange J interactions. This high-fidelity CNOT gate has an error of about 10^{-6}, below the error threshold required for fault-tolerant quantum computation, and its operation time of 100ns is about 3 times faster than 297ns of the proposed global control scheme. It also relaxes significantly the stringent distance constraint of two neighboring donor atoms of $10 \sim 20$nm as reported in the original Kane's proposal to about 30nm in which surface A and J gates may be built with current fabrication technology. The effects of the control voltage fluctuations, the dipole-dipole interaction and the electron spin decoherence on the CNOT gate fidelity are also discussed.

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One of the important criteria for physical implementation of a practical quantum computer is to have a universal set of quantum gates with operation times much faster than the relevant decoherence time of the quantum computer. In addition, high-fidelity quantum gates to meet the error threshold of about 10^{-4} (recently shown to be about 10^{-3} in [1]) are also desired for fault-tolerant quantum computation (FTQC). There have been several different approaches in optimal control of quantum gate operation problems [2, 3, 4]. This work focuses on finding control parameter sequence in near time-optimal way using the gradient ascent pulse engineering (GRAPE) [2] approach for a high-fidelity CNOT gate in Si:P based donor spin quantum computer architectures [5, 6, 7, 8] where the electron spin is defined as qubit [9]. The GRAPE [2] approach partitions a given time into several equal time steps, and in each time step of the sequence, the amplitudes of control parameters are set to be constant. For a desired operation, we can define the trace fidelity between the desired operation and the unitary operation from the sequence. Since we can calculate the derivative of fidelity with respect to the control amplitudes (gradient ascent) in each step, we will be able to obtain, given the required fidelity, the near time-optimal control sequence numerically. Recently, the GRAPE algorithm has been applied to the coupled Josephson qubit quantum computing [4], and the numerically optimal control time for a CNOT gate is found to be 55ps [4] instead of 255ps in Ref. [10].

The architecture of Si-based donor spin quantum computer [5, 6, 7, 8] is composed of ^{31}P atoms doped in a purified ^{28}Si host where each phosphorus has an electron spin and a nuclear spin. In a constant magnetic field B_0 applied in the $\hat{z}$ direction, the single-qubit Hamiltonian can be written as $H = g_e\mu_B B_0\sigma_z^e/2 - g_n\mu_n B_0\sigma_z^n/2 + A\boldsymbol{\sigma}^e\cdot\boldsymbol{\sigma}^n$, where the effective electron g-factor in Si $g_e = 2$, the g-factor for a ^{31}P nuclear spin $g_n = 2.26$, and the hyperfine interaction $A \approx 1.21\times10^{-7}$eV. According to numerical calculations [11], it may be possible to vary the hyperfine interaction with A-gate voltage by up to $\approx 50\%$ before the donor electron is ionized. Similar to the globally controlled electron spin quantum computing scheme [9], we apply a microwave (MW) magnetic field B_{ac} to allow for x-axis rotations and also always keep the B_{ac} field on as it may not be easy to control and turn on/off the B_{ac} field quickly at the precise times in experiments. If we initialize the nuclear spins to the spin up state [12], we can use the energy states of $|\uparrow_e\uparrow_n\rangle$ and $|\downarrow_e\uparrow_n\rangle$ as a qubit [9]. Following Ref. [9], by defining $\omega(A) = \Delta E(A)/\hbar$, where $\Delta E(A) = g_e\mu_B B_0 + 2A + [2A^2/(g_e\mu_B B_0/2 + g_n\mu_n B_0/2)]$, we obtain the reduced Hamiltonian in the frame rotating with the MW field

$$\tilde{H} = \hbar\Delta\omega\,\sigma_z/2 + g_e\mu_B B_{ac}\sigma_x/2, \tag{1}$$

where $\Delta\omega = \omega(A) - \omega_{ac}$, and ω_{ac} is the angular frequency of the MW field B_{ac}. We tune ω_{ac} to be the electron spin resonance frequency obtained when no voltage is applied to the corresponding A gate, i.e., $\omega_{ac} = \omega(A_0)$. Then the qubits will effectively rotate around the x-axis when $\Delta\omega = 0$ (or equivalently $A = A_0$), and around an axis which is slightly tilted when $\Delta\omega \neq 0$ (or $A \neq A_0$) described by Eq. (1).

The effective reduced two-qubit Hamiltonian, approximated from assuming that the nuclear spins are frozen out to be always up, in the rotating frame is then

$$\tilde{H} = \hbar\Delta\omega_1\sigma_z^1/2 + \hbar\Delta\omega_2\sigma_z^2/2 + g_e\mu_B B_{ac}(\sigma_x^1 + \sigma_x^2)/2 + J\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{2e}\,, \tag{2}$$

where J is the exchange interaction between two adjacent donor electron spins. We will use the reduced Hamilto-

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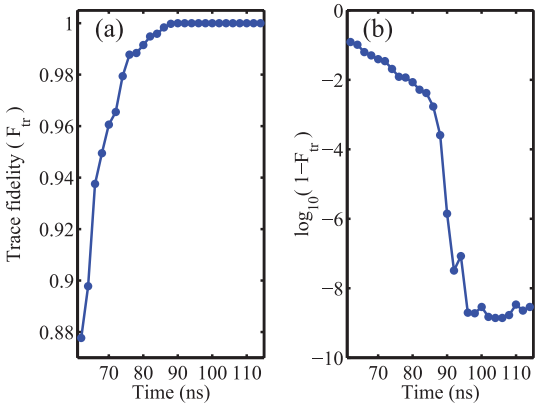

FIG. 1: (Color online) Fidelity versus time for the CNOT gate. (a) gives the trace fidelity against time, while (b) shows deviation $\log_{10}(1 - F_{tr})$ from fidelity.

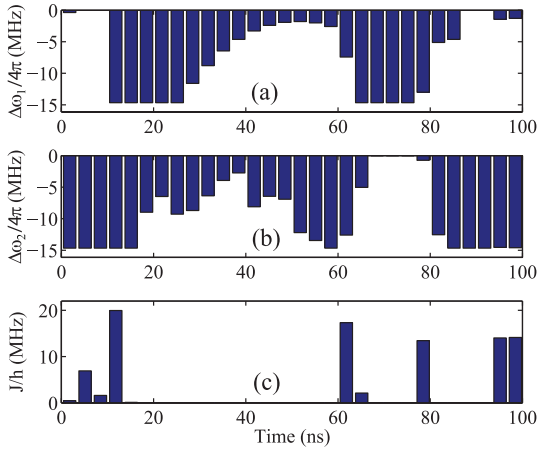

FIG. 2: (Color online) Near time-optimal CNOT gate control sequence with 30 steps in 100ns obtained using the reduced Hamiltonian. In (a) and (b), the maximum energy difference of σ_z term from detuning the hyperfine interaction is $(1/2)\Delta\omega/2\pi = -14.7$MHz. In (c), the maximum electron-electron exchange energy is $J/h = 19.96$MHz.

nian to obtain control sequences by optimizing the fidelity of CNOT gate operations using the GRAPE approach. Simulations on the full two-qubit Hamiltonian,

$$\begin{aligned} H &= g_e\mu_B B_0(\sigma_z^{1e} + \sigma_z^{2e})/2 - g_n\mu_n B_0(\sigma_z^{1n} + \sigma_z^{2n})/2 \\ &+ g_e\mu_B B_{ac}\cos\omega_{ac}t(\sigma_x^{1e} + \sigma_x^{2e})/2 + A_1\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{1n} \\ &+ g_e\mu_B B_{ac}\sin\omega_{ac}t(\sigma_y^{1e} + \sigma_y^{2e})/2 + A_2\boldsymbol{\sigma}^{2e}\cdot\boldsymbol{\sigma}^{2n} \\ &- g_n\mu_n B_{ac}\cos\omega_{ac}t(\sigma_x^{1n} + \sigma_x^{2n})/2 + J\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{2e} \\ &- g_n\mu_n B_{ac}\sin\omega_{ac}t(\sigma_y^{1n} + \sigma_y^{2n})/2\,, \end{aligned} \tag{3}$$

with the control sequences found will also be performed for error comparison.

Since the B_{ac} field is always on in this scheme, electrons will undergo a rotation around the x-axis when there are no voltages applied on A gates, i.e. $\Delta\omega = 0$, with an angular frequency of $\Omega_0 = g_e\mu_B B_{ac}/\hbar$. While the target electrons perform a particular unitary operation within time t, every spectator qubit will rotate around the x-axis with an angle of $\theta_x = \Omega_0 t$. If θ_x does not equal to $2n\pi$ where n is integral, another correction step will be required for the spectator qubits. Thus it will be convenient to choose the operation time, $t = 2n\pi/\Omega_0 = 2n\hbar\pi/(g_e\mu_B B_{ac})$, such that there is no need for correction for spectator qubits. The B_{ac} field is usually very small compared with the B_0 field. For a given time t, we choose $n = 1$ in the reduced and full Hamiltonian simulations. In this case, when the control duration is 100ns and $n = 1$, the strength of B_{ac} is 3.56×10^{-4}T.

We first try different piecewise constant control steps and numerically calculate in the GRAPE approach the fidelity (error) against the time needed to implement a CNOT gate with stopping criteria of error in the optimizer set to 10^{-9} in order to economize the simulation time. Here, the error is defined as $1 - F_{tr}$, where F_{tr} is the trace fidelity defined as $F_{tr} = |\mathrm{Tr}\{U_D^\dagger U_F\}|^2$ with U_D being the desired unitary operator in a given time t, and U_F being the optimal unitary operator constructed by our control sequence. For each trying value of time t, we divide the sequence into 30 piecewise steps, starting with each of the initial control amplitudes (A_1, A_2 and J gates; or equivalently $\Delta\omega_1$, $\Delta\omega_2$ and J) by assigning a random value to every five steps in time and using a cubic spline to fill in the amplitudes of the intermediate time steps. The values of the control amplitudes A_1 and A_2 are varied between $A_0/2$ and A_0 [9, 11], and the value of J is varied between 0 and J_0, where J_0 is chosen for the donor separation to be around 30nm. The fidelity against time obtained from the optimization of the reduced Hamiltonian Eq. (2) is shown in Fig. 1. In Fig. 1 (b), the error is less than 10^{-8} for times longer than 100ns, and it is found that 30 piecewise constant control steps for the CNOT gate operation will be sufficient to meet the required fidelity (error) and the performance would not be improved further with more steps. With the operation time $t = 100$ns and stopping criteria of error set to 10^{-16}, we can find that the near time-optimal, high-fidelity CNOT gate control sequence has an error of 1.11×10^{-16}. The digitized sequence of controls is shown in Fig. 2. In a typical Kane quantum computer's scheme, the typical value of $J/h \approx 10.2$GHz, which requires the separation between two neighboring donors to be about $10 \sim 20$nm [5]. This sets a stringent fabrication condition to fabricate surface A and J gates within such a short distance. One of the great advantages in our scheme is that the maximum exchange energy in our simulation is only $J/h \approx 20$MHz. This corresponds to a donor separation around 30nm [5, 13]. To fabricate gates of this size is within reach of current fabrication technology.

We next apply the control sequence of the CNOT gate, obtained from the optimization of the reduced Hamiltonian Eq. (2), to the full spin Hamiltonian Eq. (3). We simulate the CNOT gate numerically with initial four different computational basis electron spin states, $|00\rangle_e$,

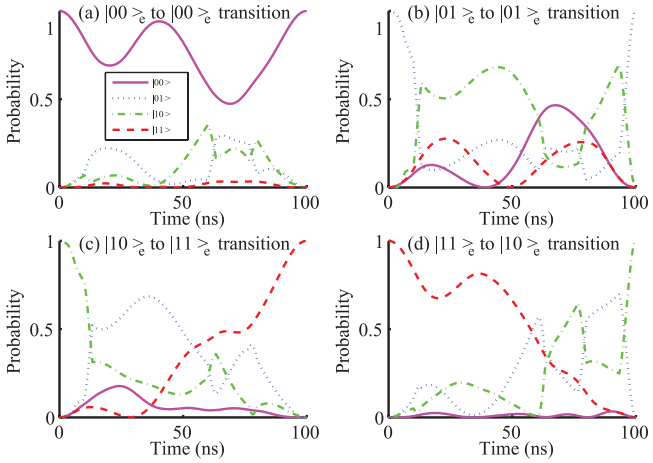

FIG. 3: (Color online) Time evolution of the CNOT gate in the rotating frame, simulated using the full Hamiltonian with 4 different initial electron-spin input states. All the nuclear spins are initially spin-up.

$|01\rangle_e$, $|10\rangle_e$, and $|11\rangle_e$, but the same nuclear spin-up state, where $|0\rangle_e$ means the electron spin is up. The final reduced electron density matrix is defined as the composite density matrix traced over all the nuclear spin states. The errors of the full Hamiltonian CNOT gate operations with the four input electron spin basis states evolving to their correspondingly expected output electron spin states are shown in Table I. Here the error is defined as $1-P$, where P is the probability that the qubits are in our desired quantum state after the CNOT operation. The time evolutions of the states of the CNOT gate are shown in Fig. 3. The error are about 10^{-6} which are below the error threshold 10^{-4} (10^{-3} in [1]) required for FTQC. Most of the errors result from the accuracy of the second-order approximation in A of Eq. (2) since the hyperfine interaction A would cause both electron spins and the nuclear spins to flip in the full Hamiltonian (3). The CNOT gate operation time of 100ns is about 3 times faster than the globally controlled electron spin scheme [9] of 297ns [in [9], the indicated CNOT time is 148ns that is due to a factor of 2 missing in the denominator of their Hamiltonian Eq. (6)]. The error probabilities that nuclear spins may flip after the CNOT gate operation for the four input electron states are around 10^{-6} (see Table I). If we repeat the CNOT process N times by simply inputting the same pure electron state $|ij\rangle$ but not reinitializing the nuclear state each time, the errors of the CNOT gate operations will accumulate. The numerical results indicate that in the worst case of the electron spin input state $|10\rangle_e$, after around 60 (250) times of operations, the error sums up to 1.03×10^{-4} (0.79×10^{-3}). Therefore in order to maintain FTQC, one has to reinitialize the nuclear spin state before about 60 (250) times of operations.

Although the exchange interaction dies off exponentially with distance, the dipole-dipole interaction that couples every pair of electronic spins in the system only dies off as $1/d^3$, where d is the distance between two qubits. The dipole-dipole interaction Hamiltonian can be written as

$$H_D = D\left[\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{2e} - 3(\boldsymbol{\sigma}^{1e}\cdot\hat{n})(\boldsymbol{\sigma}^{2e}\cdot\hat{n})\right] , \qquad (4)$$

where $D=\frac{\mu_0\gamma_e^2\hbar^2}{16\pi d^3}$ is the dipolar interaction energy, $\gamma_e=\frac{g_e e}{2m_e}$ is the gyromagnetic ratio of the electrons, and $\hat{n}$ is the unit vector in the direction joining the two electrons. In our scheme, the separation of the two donor qubits is around 30nm, and thus the corresponding $D\approx 1.98\times10^{-12}$eV, which is still five orders of magnitude smaller than the exchange energy J used in our scheme. We simulate the optimal control sequences obtained previously with the full Hamiltonian plus the dipole-dipole interaction Hamiltonian to see its effect. Since the first term in Eq. (4) has the same form as the exchange energy, we may combine this term with exchange energy. So what we really need to care about is only the second term of Eq. (4), which becomes $H'_D=-3D{\sigma_y}^{1e}\otimes{\sigma_y}^{2e}$ with the donors aligning along the $\hat{n}=\hat{y}$ axis. The fidelities of the simulation results are slightly worse than the case without dipole-dipole interaction, but they are almost the same and the errors are still below the error threshold 10^{-4} (10^{-3} in [1]) required for FTQC. So the dipole-dipole interaction may dominate for larger separations, but it is still too small to decrease significantly the fidelity of the CNOT gate operation.

Since we apply voltages on the A and J gates to control the strengths of hyperfine interaction and exchange interaction, there might be noise induced from the (thermal) fluctuations in the control circuits, which then cause the uncertainties of the control parameters and decrease the fidelity of a specific operation. To analyze the decrease of fidelity due to these uncertainties, we model the noise on the control parameters A_1, A_2 and J as independent white noise with Hamiltonian written as $H_N=\Gamma_A\xi_1(t)\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{1n}+\Gamma_A\xi_2(t)\boldsymbol{\sigma}^{2e}\cdot\boldsymbol{\sigma}^{2n}+\Gamma_J\xi_3(t)\boldsymbol{\sigma}^{1e}\cdot\boldsymbol{\sigma}^{2e}$, where the mean of the continuous time random processes $\langle\xi_i(t)\rangle=0$, the correlation functions $\langle\xi_i(t)\xi_j(t')\rangle=\delta_{ij}\delta(t-t')$, and Γ_A^2 and Γ_J^2 are the spectral densities of the noise signals, which have the dimension of $(\text{energy})^2/\text{Hz}$.

TABLE I: Summary of the CNOT gate errors.

Input state, $\lvert kj\rangle_e\otimes\lvert00\rangle_n$	Expected output state, $\lvert ij\rangle_e\otimes\lvert00\rangle_n$	Error $(1-P)^a$	Probability that nuclear spins flip^b
$\lvert00\rangle_e\otimes\lvert00\rangle_n$	$\lvert00\rangle_e\otimes\lvert00\rangle_n$	1.80×10^{-8}	1.57×10^{-7}
$\lvert01\rangle_e\otimes\lvert00\rangle_n$	$\lvert01\rangle_e\otimes\lvert00\rangle_n$	1.80×10^{-7}	2.00×10^{-7}
$\lvert10\rangle_e\otimes\lvert00\rangle_n$	$\lvert11\rangle_e\otimes\lvert00\rangle_n$	1.92×10^{-6}	1.93×10^{-6}
$\lvert11\rangle_e\otimes\lvert00\rangle_n$	$\lvert10\rangle_e\otimes\lvert00\rangle_n$	1.20×10^{-6}	1.56×10^{-6}

[a] The output reduced density matrix of the electron spins is obtained by tracing over all the nuclear states.

[b] Here, we trace the total output density matrix over the electron spin states to obtain the reduced density matrix for the nuclear spin states to compute the flipping probability.

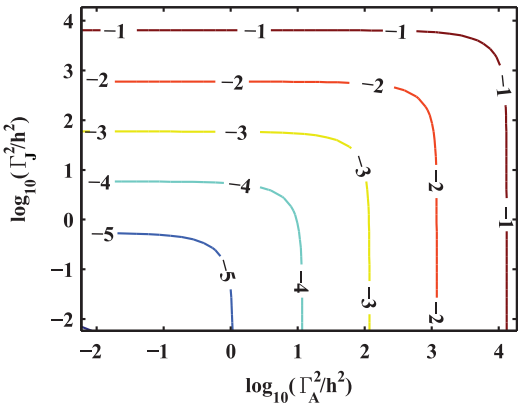

FIG. 4: (Color online) Contour plot of logarithmic errors simulated under different spectral densities Γ_A^2 and Γ_J^2 of the white noise signals on the control amplitudes of A and J of the full Hamiltonian. The unit of Γ_A^2/h^2 and Γ_J^2/h^2 in the plot is Hz and both of the axes are also in logarithmic scales.

We simulate the optimal control sequence in the presence of the white noise through the effective master equation approach [14]. The contour plot of the logarithmic errors of the full-Hamiltonian simulation results due to the white noise is shown in Fig. 4. To satisfy the error threshold 10^{-4} (10^{-3} in [1]) of FTQC, the spectral densities, Γ_J^2/h^2 and Γ_A^2/h^2, have to be smaller than 6.2Hz and 13Hz (63Hz and 125Hz), respectively. This precision of control should be achievable with modern electronic voltage controller devices. For example, it was stated in [5] that the spectral density of the gate voltage fluctuations for good room temperature electronics is of order of $10^{-18}\mathrm{V}^2/\mathrm{Hz}$, comparable to the room temperature Johnson noise of a 50 Ω resistor. At a particular bias voltage, the gates have a frequency tuning parameter $\alpha = df/dV$, estimated to be $10 \sim 100$ MHz/V [5]. Therefore, the spectral density of energy fluctuations of the control parameters for good room temperature devices can be estimated to be $10^{-4} \sim 10^{-2}$Hz that is still much smaller than 6Hz required by the error threshold of 10^{-4}.

The decoherence time T_2^e for P donor electron spin in purified Si has been indicated experimentally [15] to be potentially considerably longer than 60 ms at 4K. It has been shown [8] that the two-qubit gate fidelity of Kane's quantum computer is limited primarily by the electron decoherence time, e.g., a typical error of CNOT is 8.3×10^{-5} with operation time of 16μs for a simple dephasing model of $T_2^e = 60$ms. In our scheme, the CNOT gate time is much faster and we expect the decoherence effect may decrease the fidelity less. The error with decoherence can be estimated to be $1 - F_r e^{-t/T_2}$, where F_r and t are the trace fidelity and operation time of the gate, respectively. For this simple estimate, the error is about 2.7×10^{-6}, below the error threshold of 10^{-4} (10^{-3} in [1]).

In summary, we have applied the GRAPE approach to find the near time-optimal, high-fidelity CNOT gate control sequence. A great advantage of the CNOT gate sequence is that the maximum value of the exchange interaction is $J/h \approx 20$MHz which is about 500 times smaller than the typical value of 10.2GHz in [5, 7, 8, 9], and yet the CNOT gate operation time is still about 3 times faster than in [9]. This small exchange interaction relaxes significantly the stringent distance constraint of two neighboring donor atoms of about $10 \sim 20$nm as reported in the original Kane's proposal [5] to about 30nm. To fabricate surface gates within such a distance is within reach of current fabrication technology. Unlike traditional decomposition method that decomposes general gate operations into several single-qubit and some interaction (two-qubit) operations in series as the CNOT gate in [9], the GRAPE optimal control approach is in a sense more like parallel computing as single-qubit (A_1 and A_2 both on) and two-qubit (J on) operations can be performed simultaneously on the same qubits in parallel (see Fig. 2). As a result, the more complex gate operation it is applied, the more time one may save, especially for those multiple-qubit gates that may not be simply decomposed by using the traditional method. So the GRAPE approach may prove useful in implementing quantum gate operations in real quantum computing experiments in the future. We acknowledge supports from NSC under Grant No. 97-2112-M-002-012-MY3, from NTU under Grants No. 97R0066-65 and 97R0066-67, and from the NCTS focus group program. We are grateful to NCHC for computer time and facilities.

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clear spins in the spin-up state. Alternatively, we may read out the electron spin state (e.g. as described in [9]) or wait until the electron spins relax to the spin-down ground state, then apply MW and rf pulse to initialize the electron spins in the spin-up state and then to swap the nuclear and electron spin states. According to our simulations, the error in the initial nuclear spin-up polarization should be kept smaller than 10^{-4} (or 10^{-3}) in order to maintain FTQC.

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